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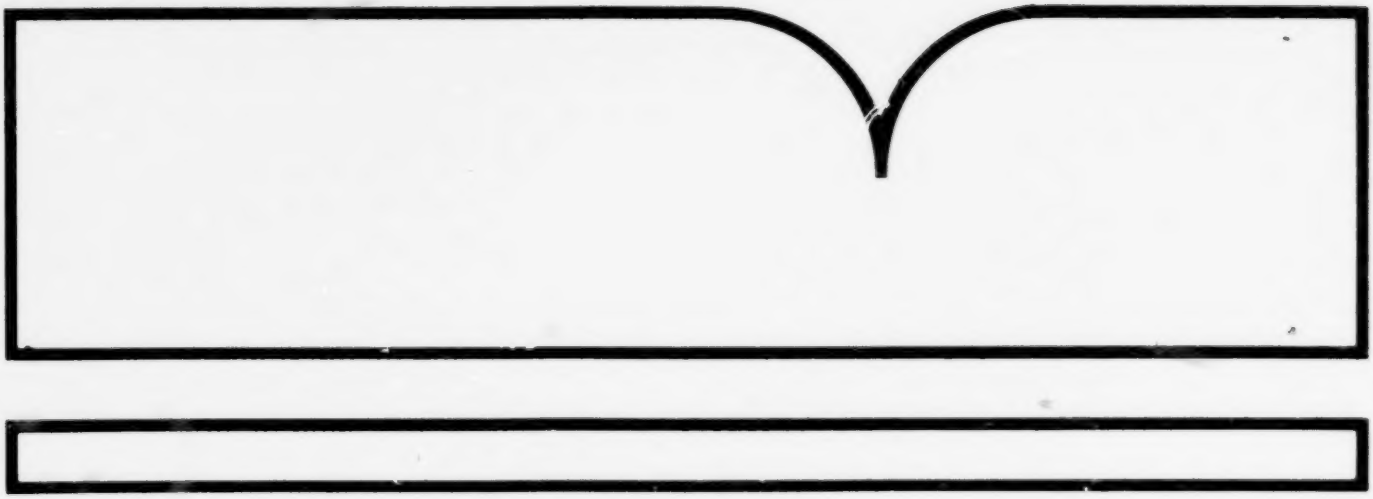

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THE USE OF WATER QUALITY MODELS IN MANAGEMENT DECISION MAKING

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ABSTRACT

The use of water quality models in three management contexts is described: screening, planning, and design. Screening models are illustrated by describing a methodology applicable to large areas of land and another applied to a large number of chemicals. The application of models in a planning context is illustrated by a local planning agency's use in developing nonpoint source control strategies and by the federal government's use in assessing potential exposure to a pesticide. Development of design criteria is illustrated by summarizing the long history of model use to develop effluent limits in the Holston River basin (Tennessee).

KEYWORDS

Water quality; mathematical models; management decisions; planning; pesticides; hazardous wastes.

INTRODUCTION

The use of water quality models in environmental management decision making can be considered in three contexts: screening, planning, and design. Although the distinctions between these categories are blurred, they are convenient in discussing applications. Generally, the screening models are the simplest, often employing manual calculations or simple computer models. Their primary use is the rapid identification of problem areas that may require detailed analysis with more sophisticated methodologies. Two examples of screening models will be discussed. Planning models involve an intermediate level of sophistication and are generally used to answer more specific questions. These models, for example, might identify pesticide application strategies that best protect aquatic life or land use controls for guarding against eutrophication in reservoirs. Design models usually address site-specific questions such as effluent limits for an industrial discharger that will meet water quality standards in a river.

Screening Models

Often, there is a requirement in water quality management to assess either an extensive geographical area or a large number of chemicals. In response,

screening methodologies have been developed to rapidly identify potential problem areas. More detailed analysis may then be performed on the problem areas and/or problem chemicals.

Such a methodology was developed for the U.S. Environmental Protection Agency (EPA) to use in the nondesignated 208 areas as defined in the Clean Water Act (PL92-500). For the most part, these areas include all land outside major U.S. metropolitan areas.

Water Quality Assessment: A Screening Method For Nondesignated 208 Areas (Zison, Haven and Mills, 1977) is designed for preliminary screening of surface water quality problems from both point and nonpoint sources. Estimation techniques are included for rivers, impoundments and estuaries. Biochemical oxygen demand, dissolved oxygen, temperature, sediment accumulation and eutrophication problems are addressed. The analyses are designed to be performed with, at most, the assistance of a desk top calculator and with a minimal amount of data input. Results, of course, are only approximations but are designed to be conservative.

The methodology is a collection of diverse techniques presented in an orderly fashion with particular emphasis on consistency. It begins with an identification of basic data needs and sources. Wasteload estimation techniques for both point and nonpoint sources are included. Typical pollutant loads for municipal and industrial source categories are given but, of course, actual data are preferred. The estimation of rural nonpoint source loads is based on a handbook developed for the EPA (McElroy and co-workers, 1976). The methodology relies on sediment loads calculated from the U.S. Department of Agriculture's Universal Soil Loss Equation. Phosphorus, nitrogen and organic matter loads are then assumed to be correlated with sediment. Pollutants in urban runoff are estimated using the techniques described by Amy and colleagues (1974). This method assumes that only runoff from street surfaces contributes to urban nonpoint pollution.

Streams and rivers are analyzed using steady-state mass balance techniques assuming plug flow and first order decay where applicable. Analyses for temperature, biochemical oxygen demand, dissolved oxygen, nutrients and conservative substances are included. Eutrophication potential is assessed using nitrogen-phosphorus ratios.

Problems addressed in the lake analysis include thermal stratification, sediment accumulation, eutrophication potential, and hypolimnitic dissolved oxygen. The thermal stratification analysis is based on a complex reservoir model that was run for a range of climatic conditions, geometries, mean hydraulic residence times, and mixing conditions. These properties were previously determined through a sensitivity analysis. The user is asked to determine the scenario that best fits his own situation and examine the results from the reservoir model. Sedimentation assessments are based on an empirical approach relying on observations in the United States. An annual nutrient budget approach, assuming phosphorus as the limiting nutrient, is used for determining eutrophication potential. The hypolimnitic dissolved oxygen model is a simplified approach relying on BOD loadings and benthic demand.

Estuarine analysis utilizes the tidal prism approach. A preliminary assessment is applied to determine whether hand calculations are appropriate or whether the problem requires a more sophisticated approach. Constituents that can be addressed using this method include dissolved oxygen and biochemical oxygen demand, temperature, coliforms, sediment accumulation, and conservative substances. The analysis begins with an assessment of flushing times;

dispersion coefficients and resulting distribution patterns for pollutants are then calculated. The next step examines sedimentation and, finally, simplified techniques for calculation of thermal discharge dispersion are described.

The output of the overall analysis is identification of marginal and critical areas for additional study. These areas may then be analyzed using more sophisticated techniques and site-specific data. To test its validity, the methodology has been applied to two relatively data-rich areas--the Sandusky River Basin in Ohio and the Chesapeake Bay Watershed (Davis, Snyder and Nebgen, 1981; Dean, Hudson and Mills, 1981). These studies showed both strengths and weaknesses in the methodology. An update and expansion of the methodology is underway, with improved techniques being incorporated where possible. A significant addition to the methodology will be procedures for estimating fate and transport of toxic organic substances. A primary strength of the methodology is its relative simplicity and the ease with which basic calculations are made. A fundamental, and probably uncorrectable, weakness is the need to accumulate and manipulate large amounts of data. In general, the river methods were the most accurate followed by estuaries and then impoundments. A qualitative assessment of the methodology is given in Figs. 1-3. Fig. 1 shows results to be good to excellent for rivers at low flow but only fair to good at higher flows. For an impoundment (Fig. 2), results were good to excellent for temperature, sediment and total nutrients, but oxygen and oxygen demand predictions were only fair to good. The estuary comparison (Fig. 3) produced mixed results but, again, predictions were better at lower flows. The level-of-effort required to perform the screening analysis has been estimated at one to three man-months for an application such as performed in the validation study.

Another requirement for screening models may arise when the environmental fate of a large number of chemicals must be assessed to determine potential exposure concentrations. Such an assessment has been described by Falco and co-workers (1982). The Resource Conservation and Recovery Act of the U.S. Congress required an evaluation of the potential for chemicals to contaminate both subsurface and surface waters after disposal and subsequent release from landfills and lagoons. A procedure was developed that estimates movement and degradation of chemicals based on a compound's physical and chemical properties and typical environmental conditions in groundwater, rivers, ponds and reservoirs. The procedure was used to evaluate 193 compounds expected to be found in solid wastes from 75 manufacturing operations.

The mathematical model employs a simple mass balance technique that routes a pollutant through a series of typical environments. It is conceptually similar to, but much less sophisticated than, the Exposure Assessment Modeling System (Burns and Cline, 1982). Release rates from landfills (per unit surface areas) and lagoons (per unit length adjacent to a river) were estimated by assuming a constant recharge rate and an infinite source of chemical. Leachate concentrations were assumed to be limited by either the solubility of the compound or by the equilibrium concentration obtained by partitioning between sorbed solid phase and dissolved material. The choice of the limiting process was made based on whether the compound was a major constituent of a waste stream or merely a small fraction of the total.

The rate of transport of a chemical through groundwater was assumed to be limited by the hydraulic conductivity of the soil and not by mass transport through the boundaries of containment facilities. The procedure also assumed that soil sorptive capacity had been reached and that steady-state concentration profiles had been achieved. Hydrolysis was the only degradation process considered in groundwater and it was assumed to be adequately approximated by a

Figure 1. Water Quality Simulation Results Summary for Rivers

	System	
	Sandusky	Patuxent
Low Flow		
Temperature	●	●
BOD	✲	●
Dissolved Oxygen	●	●
Coliforms	✲	✲
High Flow		
Sediment	◐	
BOD		
Total N		
Total P	◐	

Key:
- ● Results good to excellent
- ◐ Results fair to good
- ✲ Simulation performed, no comparative data available
- (blank) No simulation performed

Figure 2. Water Quality Simulation Results Summary for Impoundments

	Occoquan
Impoundments	
Temperature	●
BOD	◐
Dissolved Oxygen	◐
Sediment	●
Total N	●
Total P	●

Key:
- ● Results good to excellent
- ◐ Results fair to good

Figure 3. Water Quality Simulation Results Summary for Estuaries

	System		
	Chester	Patuxent	Ware
Low Flow			
BOD	◐		◐
Coliforms	✲		
Total N		●	●
Total P		●	
High Flow			
Sediment	✲		◐
BOD	○		○
Total N	◐	✲	◐
Total P	✲	✲	◐

Key:
- ● Results good to excellent
- ◐ Results fair to good
- ○ Results poor to fair
- ✲ Simulation performed, no comparative data available
- (blank) No simulation performed

first order rate equation. For landfills, the movement of water was estimated based on a range of reported recharge rates; for lagoons, estimates were based on an assumed location 100 meters from a receiving water.

Three types of receiving waters were considered--rivers, ponds and reservoirs, and a range of environmental conditions and parameters characteristic of each type was estimated. For each set of environmental conditions, estimates of the fraction volatilized, degraded, advected, bioaccumulated and sorbed to suspended sediments was made. Estimates of the fraction settled in ponds and reservoirs were also made. Major degradation processes considered include volatilization, bioaccumulation, hydrolysis, photolysis, oxidation and bacterial degradation. Sorption to suspended material was assumed to be instantaneous and totally reversible.

Environmental conditions were chosen to represent a range of typical environments found in the United States. The specific chracteristics estimated included travel times, reaeration rates, bulk sediment concentration, sediment trap efficiency, sediment organic matter content, and fish standing crop and growth rate. In the analysis of the 193 compounds, the physical and chemical properties were obtained from standard references or estimated using structure-activity relationships. The properties considered included solubility, molecular weight and octanol/water partition coefficient. Rate constants for hydrolysis, microbial degradation, photolysis, oxidation were estimated and summed to provide an overall degradation rate. In some cases, only an overall degradation rate was known. In the analyses, only limited data were available, much of which were qualitative.

For each compound, a range of loading estimates was made and for each environment a range of estimates of the fate of each compound was made. Qualitative descriptors of "low," "significant," and "high" were assigned to describe the potential for the compound to be sorbed, transported, degraded, volatilized or bioaccumulated. A computer program was written to access the environmental and compound characteristic data files, perform calculations, assign descriptors, and type a text that used the descriptors to qualitatively describe the potential exposure of each chemical. After the initial predictions, a sensitivity analysis on various model parameters was done. The analysis showed the degradation rate coefficients to be the most sensitive parameter with the volatilization rate and partition coefficient showing less overall sensitivity.

Finally, observations of occurrence of a compound as reported in EPA's Distribution Register of Organic Pollutants in Water (Water DROP) (Garrison and co-workers, 1979) were reported with model predictions. Observations of occurrence are strong evidence of compound persistence and, in general, the potential for human exposure can be considered high for any compound reported in Water DROP. Conversely, a compound's absence from Water DROP does not guarantee its absence from ambient waters but may merely reflect a lack of monitoring or, even, an adequate analytical method. This comparison was done in an attempt to check for consistency between model predictions of potential exposure and observations of the compounds.

Planning Models

In contrast to the relative simplicity and ease of application of screening models, planning models are more sophisticated and require significant effort to use. Probably one of the most sophisticated uses of planning models by a public agency in the United States was conducted by the Northern Virginia Planning District Commission (NVPDC). NVPDC is responsible for water quality management

planning in the Occoquan River Basin, which encompasses four counties and two cities in the Virginia suburbs of Washington, DC (Fig. 4). The water supply reservoir at the mouth of the watershed currently serves more than 600,000 customers and is one of the few major water supply impoundments in the Eastern United States that is located downstream from an urban region. The application of a water quality model to develop a water quality management plan for the Occoquan Basin has been described by Bonnucelli, Hartigan and Biggers (1980).

In the late 1960s, the reservoir began exhibiting symptoms of cultural eutrophication, and in 1971 a decision was made to replace existing secondary sewage treatment plants in the basin with an advanced wastewater treatment (AWT) plant immediately upstream of the reservoir. At the same time, the Occoquan Watershed Monitoring Laboratory (OWML) was founded to establish baseline surface water quality records. The Occoquan AWT plant began operation in early summer, 1978. The AWT decision was based on the assumption that urban nonpoint pollultion would not significantly degrade the quality of Occoquan Reservoir. In the mid-1970s, it came to be recognized that urban sources can contribute significant loads. Studies were initiated in 1975 under Section 208 of the Clean Water Act to determine the magnitude of the nonpoint source problem and develop a management program. A computer-based water quality model of the Occoquan River basin was used in this planning effort. This model relied primarily on the U.S. EPA's Nonpoint Source Model (Donigian and Crawford, 1976) and the Hydrocomp Simulation Programming (HSP) model (Hydrocomp, Inc., 1976). The hydrologic and water quality processes represented by the model include the conversion of rainfall to runoff, the washoff of pollutants from the land surface, the delivery of runoff and associated pollutant loadings to receiving waters, the release of subsurface pollutants in baseflow, the contribution of sewage treatment plants to receiving waters, and the water quality response of the stream channels and reservoirs in the watershed.

The extensive data base on nonpoint pollution loadings that existed in the basin was key to the application of this sophisticated modeling approach. This data base was collected in an intensive field study carried out by NVPDC and Virginia Polytechnic Institute and State University from June 1976 through May 1977. During this study, more than 300 storm events on 21 watersheds were sampled. The data were used to calibrate the computer model and to derive relationships between land use and nonpoint pollution. Model calibrations were verified by comparing simulations of earlier time periods to data collected by the OWML. Results were judged to be quite good for the watershed hydrologic response and to adequately represent land surface loadings and instream transformations of pollutants.

The calibrated, verified model was then used to examine the long-term water quality impacts of land development patterns and best management practice (BMP) strategies. Land use patterns were projected to the year 2005 and were then used to evaluate the relative effectiveness of different urban runoff BMPs. The BMPs evaluated include source controls, discharge controls and volume controls.

Source controls are measures that reduce the accumulation of pollutant loads on the land surface. They include such techniques as land use planning, fertilizer management programs and parking lot/street sweeping programs. Discharge controls are measures that detain runoff for several hours and release it at a controlled rate. They may be as simple as detention ponds to allow adequate time for sedimentation. (The recommended design criteria for the Occoquan Basin would provide for removal of the silt size fraction.) More sophisticated discharge controls might rely on physical/chemical stormwater treatment facilities. Volume controls are measures that reduce runoff levels by diverting excess runoff into the soil profile where natural processes remove pollutants.

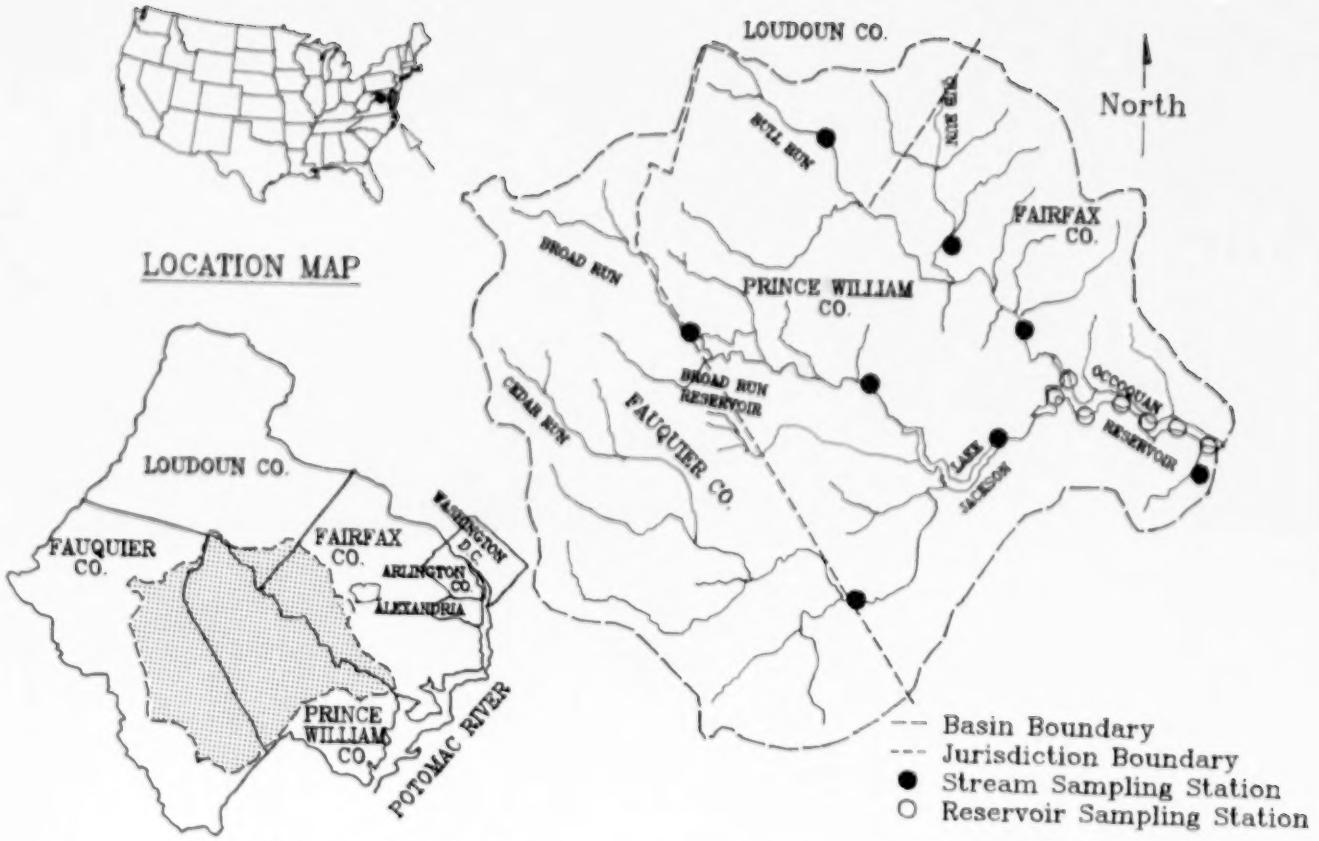

Figure 4. Generalized Map of Occoquan River Basin
after Bonnualli, et. al. 1980

Such practices as porous pavements or seepage pits are included in this class.

The modeling studies indicated that high levels of wastewater treatment alone would not be adequate to eliminate water quality problems in the Occoquan Basin. Traditional stormwater management techniques such as volume controls and modified detention basins were determined to provide adequate protection. The modified detention basin design was projected to involve a 10-20% cost increase over a conventional design. Stormwater treatment BMPs achieved the greatest reductions in pollutant loadings but the increased water quality benefits did not appear to be great enough to offset their extremely high cost.

Based upon these projections, the local governments have begun to implement urban nonpoint pollution BMPs in their areas of responsibility. All new development activities will be required to implement these practices. The application of a comprehensive water quality planning model has allowed these governments to determine cost-effective solutions to water quality problems that transcend local political boundaries.

Planning models may also be used at the regional scale. A study of fate and transport of the pesticide toxaphene to estimate potential environmental exposure is an example of such an application (EPA, 1979; Mulkey and Falco, 1980). Toxaphene is a chlorinated insecticide used for control of pests in both food and fiber crops including vegetables, feed grains, and cotton. The factors of persistence, extent of current use, geographical distribution of use, increasing rates of application required for efficacy, and high toxicity to non-target species including freshwater fish combine to pose a significant potential environmental hazard. The study was undertaken to determine the potential environmental exposure from differing application rates of the pesticide, to investigate the risk to selected freshwater species resulting from application of toxaphene on watersheds having large areas cropped to cotton, and to determine an application rate that would adequately protect aquatic life.

The factors of cotton production, rainfall and runoff combine to make the Mississippi Delta region an area where toxaphene exposure is likely to be greatest. Within this region, the Yazoo River Basin was chosen as a representative system for specific analysis (Fig. 5). A factor in the choice of the Yazoo was the existence of an extensive hydraulic and hydrologic data base developed in a recent study of sediment loadings on transport (Simons and Li, 1979).

Runoff of toxaphene from agricultural areas was simulated using the Agricultural Runoff Management Model (ARM) (Donigian and Crawford, 1977). Toxaphene is normally used as a foliar-applied formulation and has high persistence (half-life on the order of 1 year), low solubility (on the order of 1.0 mg/l), and high affinity for soil. Volatilization losses from foliage are generally recognized as a major mode of transport from cotton fields. (A foliar volatilization half-life of 22 days was used in this study.) The modeling approach used considered the initial distribution of applied toxaphene between foliage and soil, disappearance rates from both foliage and soil, response of foliar toxaphene to rainfall and defoliation, and runoff of toxaphene from the land surface. On a long term basis, approximately 5% of the toxaphene applied can be expected to appear in runoff (U.S. EPA, 1979).

Toxaphene attenuation in the stream-channel system was assumed to be first order enabling the lumping of all processes influencing toxaphene disappearance into one expression. A review of the literature indicated toxaphene was subject to only volatilization and sorption in water. Other processes such as microbial degradation may be active but the mean residence time of a few days for the

Figure 5. Yazoo River Basin, Mississippi

Figure 6. Holston River Basin
after Higgins (1978)

Yazoo River Basin makes processes having long half-lives unimportant for the instream assessment.

The transport model used to simulate instream pesticide concentrations was a simple Continuously Stirred Tank Reactor (CSTR) formulation. Lumped first-order degradation processes and sorption on fine sediment were the only processes considered in the model; interactions with bed sediment were not considered. Daily flow rates and segment water volumes were estimated using the Yazoo River Basin hydraulic and hydrologic data base. A 5-year time period using meterologic and hyurologic data from 1971-1975 was simulated. Because of the importance of suspended sediment interactions, simulations were performed for four cases differing only in their handling of instream sediment concentrations. Three cases used the observed lower 10th percentile, mean, and 90th percentile instream sediment concentrations, and the fourth case used the simulated sediment loadings from the ARM model. The ARM simulations produce edge-of-field loadings and these results could expect to be attenuated somewhat before entering a main river system. Comparisons of the simulated loadings with mean measured sediment concentrations indicated an actual delivery ratio of approximately 25%.

The predicted instream toxaphene concentrations were then analyzed using a risk assessment methodology developed for the EPA (Onishi and co-workers, 1982). The methodology used toxicity data for four species of fish--large mouth bass, bluegill sunfish, channel catfish and fathead minnow. The analysis considers both the frequency and duration of exceedance of a curve of LC50-duration values and provides an assessment of both acute and chronic toxicity. The results of the study indicated that, at the expected application rates, exposure levels of dissolved toxaphene in the Yazoo River system are high enough to cause both short and long term changes on the aquatic species examined. The results, however, were shown to be very sensitive to assumptions about instream sediment concentrations because of toxaphene's high affinity for sediment.

The results of this study are being used in EPA's Rebuttable Presumption Against Registration (RPAR) review of toxaphene. A similar application of this methodology was used in evaluation of the application for registration of a new pesticide and was partially responsible for its conditional use registration.

Design Models

Use of models in design is probably the most common application of water quality modeling in the United States. A prime example, illustrating typical interaction between the government and the discharger in the United States, is provided by a study in the Holston River in Tennessee (Fig. 6).

Studies by the Tennessee Valley Authority (TVA), beginning as early as 1937, described the Holston River in Eastern Tennessee as "seriously polluted," with later reports citing problems with industrial waste, partially treated sewage, and mercury contamination. In June and July 1969, an intensive field survey was conducted by the Federal Water Quality Administration (later to become part of the EPA), the TVA, and the Tennessee Department of Public Health (U.S. EPA, 1972). The purpose of the study was to develop recommendations for water quality management in the basin. The study found water quality to be seriously degraded by discharges of 5-day biochemical oxygen demand, nitrogenous wastes, thermal discharges, and a prolific benthic community. A mathematical model was developed to evaluate management options and develop abatement recommendations. The model considered the impacts of dischargers and aquatic macrophytes on dissolved oxygen in the river. Modeling results also made a significant contribution to subsequent negotiation between the Federal government and a

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major industrial discharger who independently modeled the river (Krenkel and Novotny, 1973). The industry's modelers reached different conclusions about appropriate pollutant discharge levels and the industry and the Federal government reached a negotiated settlement. National Pollutant Discharge Elimination System (NPDES) permits were written with the negotiated discharge limitations to be effective in July 1977.

By 1977, routine monitoring indicated substantial improvements in water quality in the Holston River (Higgins, 1978). In the summer of 1977, the EPA conducted field studies to determine compliance with the NPDES limits and to document improvements in water quality. A water quality model was again employed to determine the relative impacts of discharges and natural factors (primarily aquatic macrophytes) on dissolved oxygen in the Holston River and to evaluate further refinements in permit limitations (U.S. EPA, 1978). The QUAL-II computer code (Roesner, Monsor and Evans, 1973), which has seen wide use in the United States, was employed.

The 1977 study concluded that water quality in the Holston River had improved considerably since the 1969 study and that these improvements were the result of reductions in industrial and municipal waste discharges. The water quality model showed that approximately one-half of the observed maximum dissolved oxygen deficit was the result of waste discharges and that the remaining deficit could be attributed to the benthic community. If benthic respiration could be eliminated from the river system, the model showed that a dissolved oxygen level exceeding the standard could be maintained, thus validating the earlier predictions.

The 1977 model was used to evaluate additional water quality management options for the Holston River including the elimination of an ammunition plant discharge, the relative water quality benefits of secondary versus advanced waste treatment at the municipal discharger, and alternate permit limits at a textile mill. The model predicted a maximum improvement of 0.25 mg/l in dissolved oxygen levels under any of the proposed scenarios. In these applications, water quality models were shown to produce valid, reasonable predictions of water quality in the Holston River. The key to their effective use was a cooperative attitude and open discussions between regulators and permittees. The model also aided decision makers in making rational decisions on appropriate levels of waste treatment in the basin.

Summary

Water quality models are used for a wide range of purposes in the United States and have a history of successful application. Their applications include screening large areas or large numbers of chemicals to identify potential problem areas, development of appropriate strategies for control of pollutants, and development of effluent design criteria for specific dischargers. In many of these applications, models provide the only method for evaluating the complex interactions between pollutants and the environment. Our experience has shown, however, that these tools should be used with care and tempered with reasoned scientific judgement. Wherever possible, model results should be confirmed with independent data or analyses. A thorough and objective review of a model application can be a significant factor in the acceptance of a model's results, both in the specific application being considered and in future applications of similar models.

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